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by

**R. Bavli and H. Metiu**

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# Laser Induced Localization of an Electron in a Double-Well Quantum Structure

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**Abstract:** In this letter we integrate numerically the time dependent Schrödinger equation to investigate the use of a semi-infinite laser pulse to localize an electron in one of the wells of a double well quantum structure. Under certain conditions the system can be driven to emit strongly low frequency radiation.



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In a recent letter Grossman, Dittrich, Jung and Hänggi<sup>[1]</sup> have pointed out an interesting effect of a cw laser acting on an electron in a quartic double well. If the electron is initially localized in one of the wells, and if the laser power and frequency are chosen appropriately, the radiation field can prevent the electron from tunneling back and forth between the wells.

In this letter we investigate a more complex question: can a semi-infinite laser pulse act on a ground state electron, localize it in one of the wells, and then keep it there? Previous work<sup>[1]</sup> was concerned with maintaining the localization but not with creating it.

We study an electron with an effective mass  $m^* = 0.067 m$  ( $m$  is the electron mass) trapped in the potential shown in Fig. 1. The parameters of the potential are typical of a double quantum well<sup>[2]</sup>. As in the previous study<sup>[1]</sup> we use a potential that does not allow the electron to escape from the two well system.

The laser electron interaction is

$$V(t) = \begin{cases} e z E_0 \exp [-(t-t_0)^2/(2\tau^2)] \cos[\omega t + \delta] & t \leq t_0 \\ e z E_0 \cos[\omega t + \delta] & t \geq t_0. \end{cases} \quad (1)$$

Here  $e$  and  $z$  are the electron charge and its coordinate along an axis perpendicular to the walls of the well. The laser parameters are the frequency  $\omega$ , the rise time  $\tau$  and the phase  $\delta$ . The parameter  $E_0$  is specified by giving the photon energy flux  $I_0 = 2\epsilon c E_0^2$  for  $t > t_0$ . If  $E_0$  is given in StV/cm,  $c = 3 \cdot 10^{10}$  cm/sec and  $\epsilon = 1/(4\pi)$  then  $I_0$  is obtained in erg sec<sup>-1</sup> cm<sup>-2</sup>. We have not attempted to solve Maxwell equations to find the field inside the well, which should appear in the Schrödinger equation for the

electron. For the strong fields used here Maxwell's equations are nonlinear and solving them is difficult. It is thus customary to use Eq. (1) and hope that the errors are not significant as long as the laser does not excite the electromagnetic resonances of the structure.

The results reported in what follows are obtained by solving numerically<sup>[3]</sup> the time dependent Schrödinger equation for the Hamiltonian defined above. A brief description of the strategy pursued is instructive. We start first with the initial state  $|L\rangle = (|1\rangle - |2\rangle)/2^{1/2}$  which is localized in the left well.  $|1\rangle$  and  $|2\rangle$  are the two lowest energy eigenstates of the system in the absence of the laser. Then we find, by numerical experimentation, the laser power, frequency and phase for which a cw laser will keep the electron in the left well. Except for the explicit consideration of the phase  $\delta$  this part of the calculation is similar to that of Ref. 1. We find that, in the present system as in the quartic double well<sup>[1]</sup>, an electron initially located in the left well is maintained there by the action of the laser. At a laser intensity  $I_0 = 43.4 \text{ MW/cm}^2$  and a phase  $\delta = 1.5 \pi$  localization is maintained for photon energies of 104.27 (841.0  $\text{cm}^{-1}$ ), 17.18 meV (138.57  $\text{cm}^{-1}$ ), 8.295 meV (66.9  $\text{cm}^{-1}$ ), or 4.215 meV (34.0  $\text{cm}^{-1}$ ); the probability of finding the electron in the left well is never less than 75% and its average over time exceeds 90%. Prior work used  $\delta = \pi/2$  (i.e. it used  $\sin(\omega t)$  for the time dependence of the field) and did not comment on the fact that the results are dependent on the laser phase. We find that the quality of localization is good (and the same) for  $\delta = 1.5 \pi$  and  $\delta = 0.5 \pi$  and more poor for  $\delta = 0$  and  $\delta = 1.0 \pi$ .

Once we find the conditions ( laser power, frequency and phase ) which maintain the initially localized electron in its well, we start a new calculation in which the electron is initially in an eigenstate of the bare ( i.e. no laser) double well

and is exposed to a semi-infinite laser pulse. We use a pulse intensity and frequency for which the cw laser was capable of maintaining the electron localization in the previous calculation ( in which the electron was initially localized). The phase  $\delta = -\omega t_0 \pm 2n\pi$  is chosen to give a maximum electric field  $t = t_0$ . We pick a pulse rise time  $\tau$  and we calculate, by solving the time dependent Schrödinger equation, the wave function of the electron and monitor the time evolution of the probability that the electron is in the left well. We vary  $\tau$  until we find a value for which the laser localizes the electron in a well and then keeps it there.

In Fig. 2 we show the probability  $P_L(t)$  that the electron is in the left well, as a function of time. The electron started in the left well. The pulse properties are indicated in the figure. Let us examine the upper curve of Fig. 2a. The electron is initially (i.e. at  $t=0$ ) in the ground state and the wells are occupied with equal probability. The laser amplitude is a Gaussian which has a width  $\tau$ , reaches a maximum at  $t=t_0 = 3.5 \tau$  and then levels off to a constant value. The value of  $\tau$  for the upper curve in Fig. 2 is 585 fs. In the early times, when the laser intensity rises,  $P_L(t)$  undergoes wild oscillations and the electron moves from one well to another. When the pulse settles to a constant value,  $P_L(t)$  oscillates with a small amplitude around a mean value larger than 0.95. The period of these small oscillations is the laser frequency. The second graph in Fig. 2a shows that if we change the rise time from  $\tau = 585$  fs to  $\tau = 540$  fs, but keep all other parameters unchanged, the electron will be localized in the right well. We have found, for  $I_0 = 43.4$  MW/cm<sup>2</sup> and  $\omega = 138.57$  cm<sup>-1</sup>, about 20 values of the rise time  $\tau$  for which the electron is localized in one of the wells. Fewer rise times leading to localization were found when the laser frequency is 66.9 cm<sup>-1</sup>, and none for frequencies higher than 138.57 cm<sup>-1</sup>.

One is accustomed to think that spectroscopic observables are independent of the overall phase  $\delta$  of the electromagnetic field. This is indeed true for many one pulse, low intensity experiments:  $\delta$  disappears from the equations used to calculate observables. At the laser powers used in the present calculations this independence on phase no longer holds. Calculations using laser parameters (i.e. rise time, frequency and power) that localize the electron in the left well for  $\delta = -\omega t_0 \pm 2n\pi$ , localize the electron in the right well if  $\delta = -\omega t_0 \pm (2n+1)\pi$ . For the same parameters but  $\delta \neq -\omega t_0 \pm n\pi$ , the localization is very poor. A change of phase by  $\pi$  is equivalent to a change in the sign of  $z$  (see Eq. 1). As a result the operator  $P_L = \int_{-\infty}^{L/2} dz |z\rangle\langle z|$  whose expectation value gives the population in the left well is converted by the transformation  $\delta \rightarrow \delta \pm \pi$  into the operator giving the population in the right well.

Unless one works at a very low temperature the excited state  $|2\rangle$  is initially populated. For this reason we have also investigated the effect of a semi-infinite pulse in the case when the electron starts in  $|2\rangle$ . We find that a pulse having a set of parameters that localize an electron starting in  $|1\rangle$  in the left well, will localize an electron starting in  $|2\rangle$  in the right well. If the same pulse acts on an electron in thermal equilibrium the population in the left well will exceed that in the right one by a Boltzmann (or a Fermi) factor.

The extent of the trapping is rather sensitive to the parameters of the pulse. As illustrated by Fig. 2, relatively small changes in  $\tau$  (e.g. 40 fs for Fig. 2a and 147 fs in Fig. 2b) can change the localization from the left to the right well. Small deviations from the frequency required to localize the electron in the left well cause  $P_L(t)$  to drift slowly from about 0.9 to about 0.1 and back. In calculations using a photon energy

close to 17.18 meV the period of this drift is of order  $1/\Delta\omega$ , where  $\Delta\omega$  is the difference between the photon frequency used in the calculation and the frequency (i.e. 17.18 meV) at which the localization is achieved. At lower photon energies this drift is faster: if the laser frequency is close to 104.27 meV the drifting period is about three time longer than  $1/\Delta\omega$ .

We have also calculated the dipole  $\mu(t) = \langle \Psi, t | x | \Psi, t \rangle$  of the sample, where  $|\Psi, t\rangle$  is the wave function of the electron at time  $t$ . In Fig. 3 we show

$$\mu(\Omega) = \left| \int_{-\infty}^{+\infty} dt e^{-i\Omega t} W(t-t') \mu(t) \right|$$

The width and the center  $t'$  of the Gaussian window function  $W$  is chosen to cut off the values of  $\mu(t)$  at times when the pulse intensity is still rising.  $\mu(\Omega)$  has peaks of Gaussian shape ( i.e. the transform of the window function) centered at the frequencies at which the Fourier components of  $\mu(t)$  are non-zero. In Fig. 3 we show only the positions and heights of these peaks. The parameters for the laser pulse (indicated in the figure) are those that lead to localization if the initial state was the bare ground state. The transform in Fig. 3a has a large number of peaks forming two progressions: one at  $n\omega$  ( $\omega$  is the laser frequency) and the other at  $n\omega + 10.7 \text{ cm}^{-1}$ , where  $n$  is an integer. There are several striking features. The amplitudes of the terms in the progression  $n\omega$  are larger for  $n$  even. The intensity of the harmonics does not decay with  $n$  as one would expect if high order perturbation theory had any validity. For example, the intensity of the twenty second harmonic is a third of that of the Rayleigh (i.e. having the same frequency as the incident laser ) peak. Similar results are obtained for a laser frequency of  $138.57 \text{ cm}^{-1}$ , a power of  $43.4 \text{ MW/cm}^2$  and a rise time that leads to electron localization (Fig. 3b). We see two progressions at  $n\omega$



and  $n\omega - 43.37 \text{ cm}^{-1}$  (or  $n\omega + 95.2 \text{ cm}^{-1}$ ). There are substantial differences between these two cases but we still see high harmonics (the peak at  $12\omega$  is about one fourth of the largest peak which appears at the frequency of the incident light).

The behavior of the transform of  $\mu(t)$  becomes more interesting if the laser frequency is slightly off the laser frequency that would cause localization. For example, we have performed calculations at  $\omega = 148.57 \text{ cm}^{-1}$ ,  $I = 43.4 \text{ MW/cm}^2$  and a rise time that would localize the electron if the frequency was  $138.57 \text{ cm}^{-1}$ . The transform of  $\mu(t)$  in this case has peaks at  $(2n+1)\omega$ ,  $(2n+1)\omega \pm 17.77 \text{ cm}^{-1}$ ,  $2n\omega \pm 25.18 \text{ cm}^{-1}$  and  $2n\omega \pm 5.54 \text{ cm}^{-1}$ . There are no peaks at  $2n\omega$  even though an identical calculations with a laser frequency of  $138.57 \text{ cm}^{-1}$  (for which the electron is localized) has the highest peaks at  $2n\omega$ . More interesting is the appearance of a low frequency peak (at a frequency lower than that of the light) whose intensity is about four times larger than that of the Rayleigh peak (i.e. the peak at the incident light frequency). The same phenomenon occurs if the light frequency is  $10 \text{ cm}^{-1}$  lower than the localization frequency (which is  $138.57 \text{ cm}^{-1}$ ). The reason for this intense low frequency peak is that the electron population is no longer localized but drifts slowly from one well to another. This low frequency mode, in which the charge density oscillates slowly between the wells, has a higher dipole and hence a more intense emission.

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Allen, Mark Sherwin and especially with Martin Holthaus are gratefully acknowledged.

### References

- 1 F. Grossmann, T. Dittrich, P. Jung, and P. Hänggi, Phys. Rev. Lett. **67**, 516 (1991); Related work was also performed by D. Neuhauser, Coherent Destruction of Tunneling-Physical Origin (preprint); M. Holthaus, Pulse-Shape-Controlled Tunneling in a Laser Field, (preprint).
- 2 G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures* (Halsted, New York, 1988); C.W.J. Beenakker and R. Van Houten, in *Semiconductor Heterostructures and Nanostructures*, eds. G. Ehrenreich and D. Turnbull (Academic Press, New York, 1991).
- 3 J.A. Fleck Jr., J.R. Morris and M.D. Feit, Appl. Phys. **10**, 129 (1976); M.D. Feit, J.A. Fleck Jr. and A. Steiger, J. Compt. Phys. **47**, 412 (1982); M.D. Feit and J.A. Fleck Jr., J. Chem. Phys. **78**, 2578 (1984).

### Figure Captions

**Fig. 1** The potential energy felt by the electron in the absence of the laser field. The barrier height is 240 meV and its width is 45Å. The wells have about the same width as the barrier. The potential energy is :  $V(R) = \{ [(D + |D|)/2]^{1/4} - [(D - |D|)/2]^{1/4} + 1 + \exp [30(R-L/2)/L] / 1000 \}$  where  $L$  is the total length of the structure and  $D \equiv \cos (6.6R/L - 1.3\pi)$ . The horizontal lines show the lowest four eigen-energies of the electron in the absence of the laser. The broken and solid lines show the wave functions of the electron in the two lowest bare energy eigenstates.

**Figs. 2.** The time dependence of the probability  $P_L(t)$  that the electron is in the left well. The initial state is the bare ground state  $|1\rangle$ . The optical field is given by Eq. 1. The laser power when the pulse amplitude becomes constant is  $I_0 = 43.4 \text{ MW/cm}^2$ . The photon energy is a) 17.18 meV ( $138.57 \text{ cm}^{-1}$ ) and b) 8.295 meV ( $66.9 \text{ cm}^{-1}$ ). Depending on the rise time of the pulse the electron is localized in the left well ( the thin line) or in the right one ( the thick lines).

**Figs. 3** The peak positions and heights in  $\mu(\Omega)$  (see the definition given in the text). The calculation in Figs. 3 (a) and 3 (b) were performed for the parameters used in Figs.2 (a) and (b).

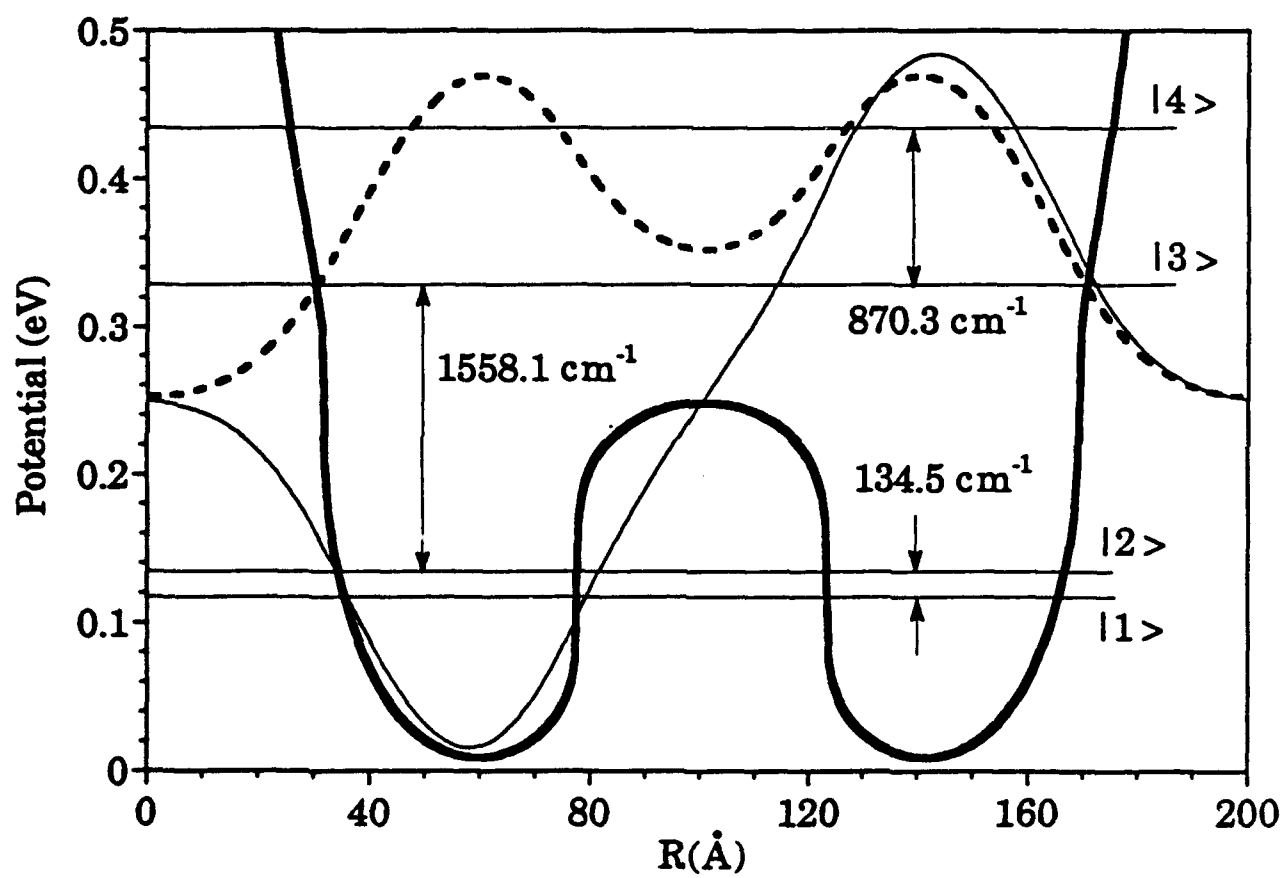


Fig. 1

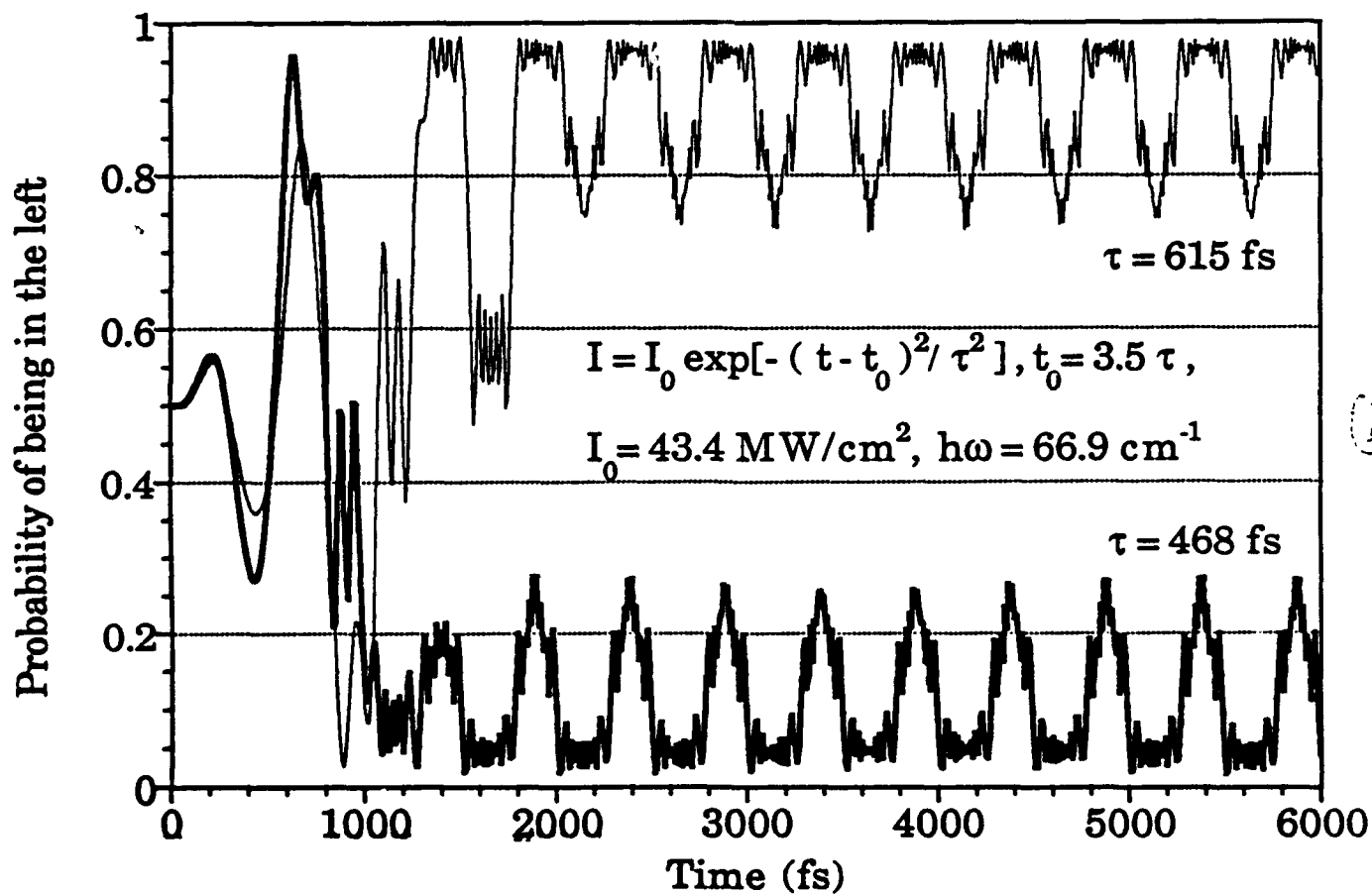
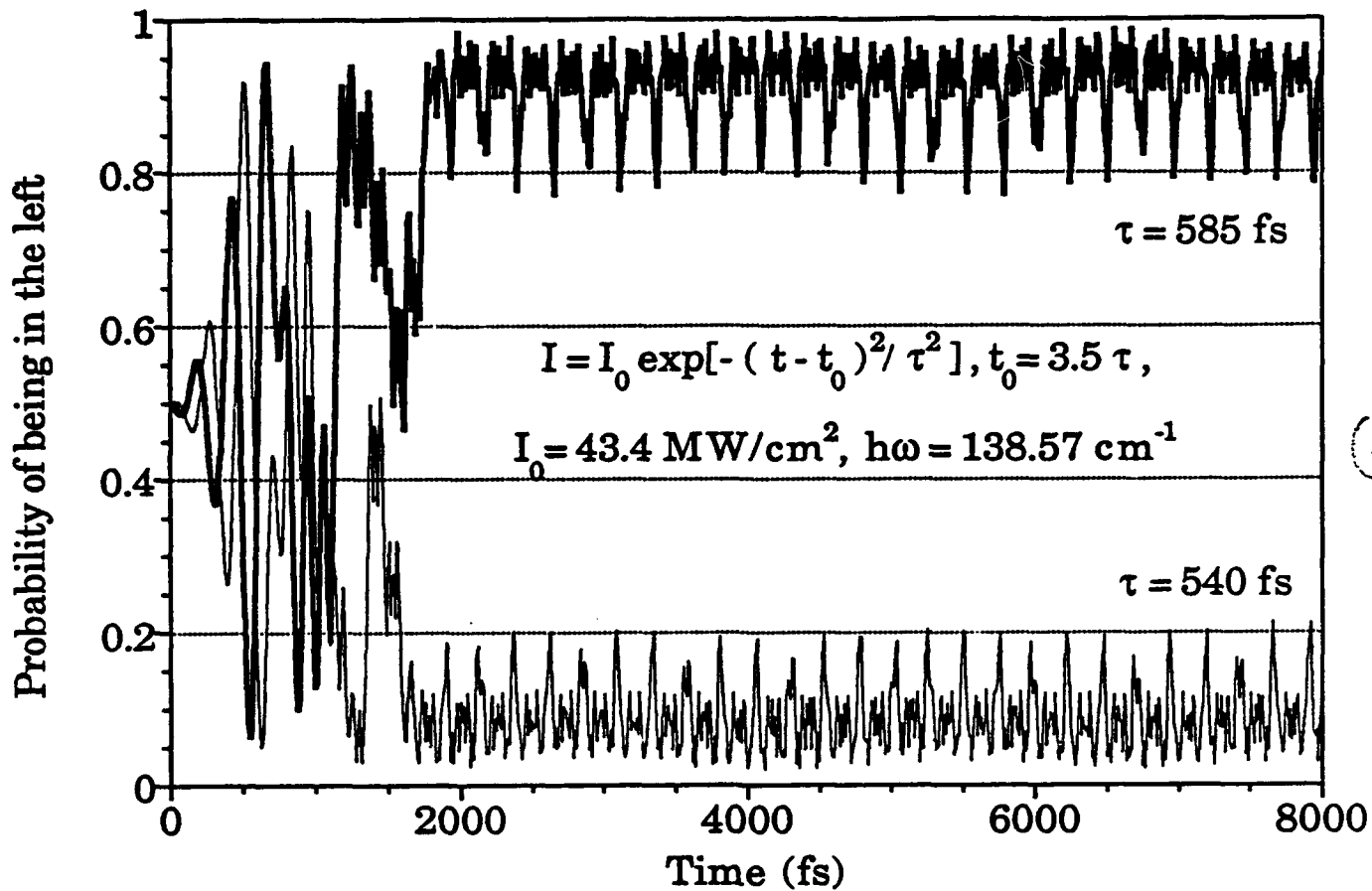


Fig 2

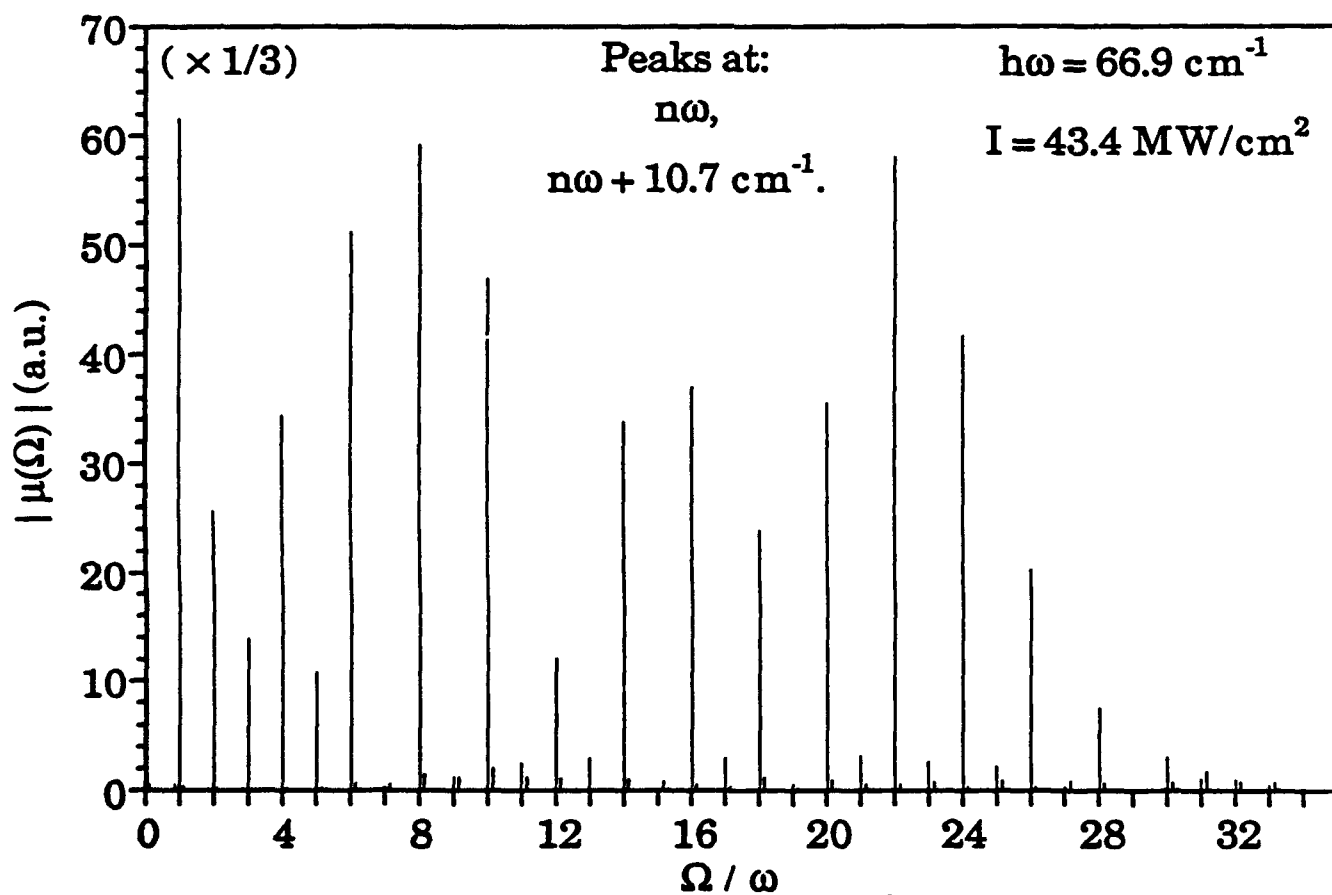
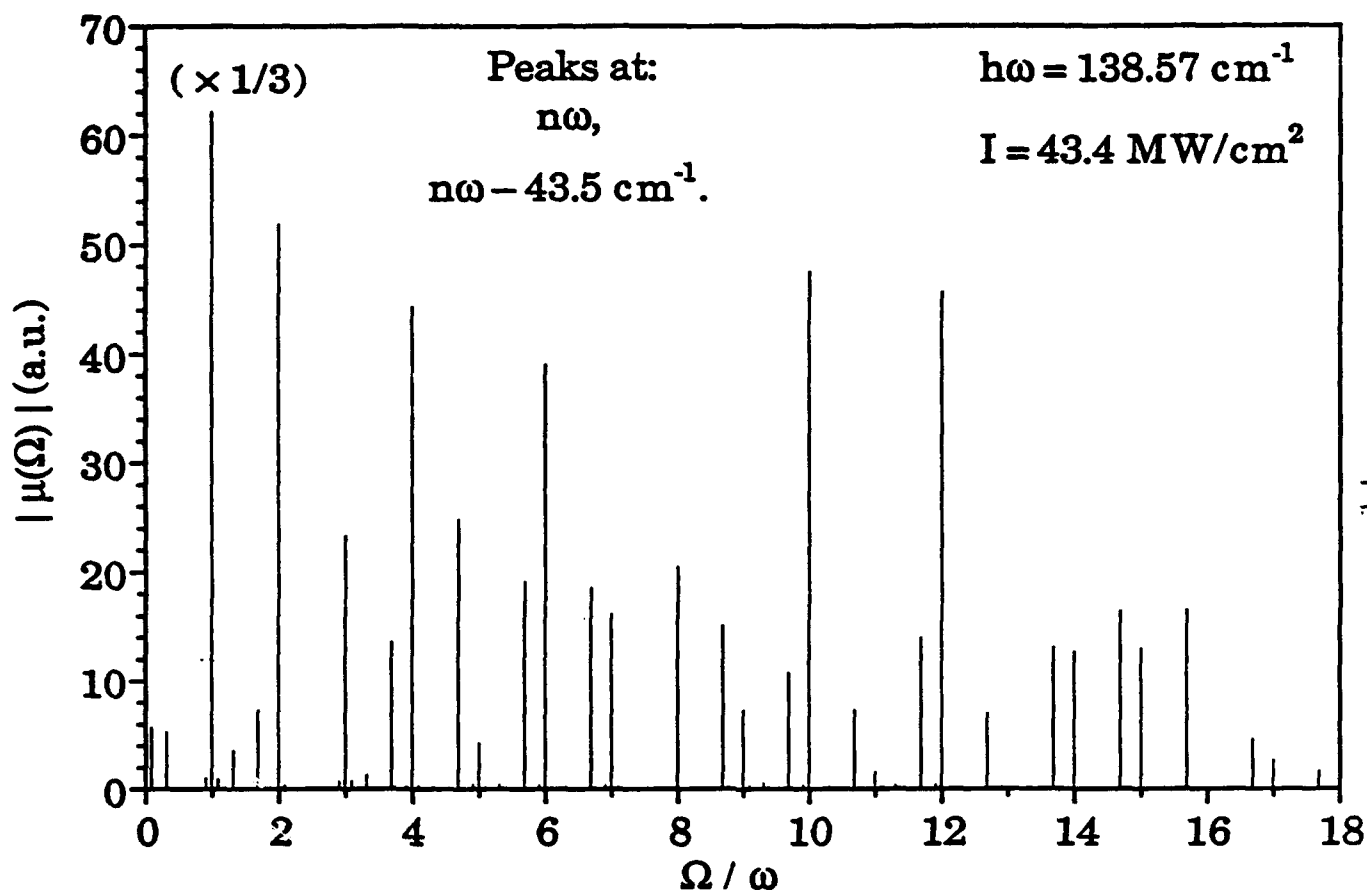


Fig. 3a

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